6.5 Least Squares Problems

Ex. Consider the system

$$\begin{aligned} 2x_1 &= 7 \\ x_1 + x_2 &= -3 \\ x_1 + 2x_2 &= 1 \end{aligned}$$

or, in matrix form

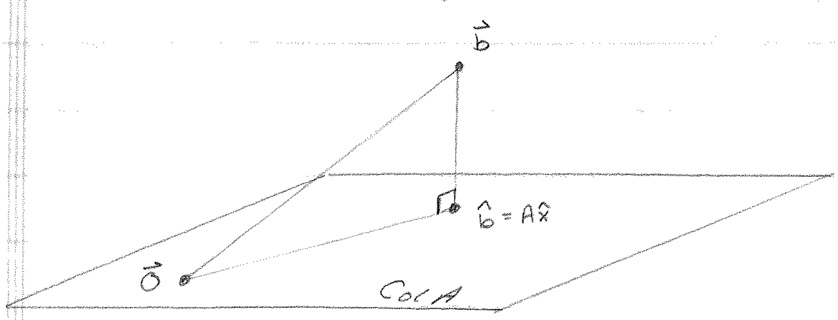
$$\begin{bmatrix} 2 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 7 \\ -3 \\ 1 \end{bmatrix}$$

We can attempt the solution various ways, but notice from the first eq. that $x_1 = 7/2$ so from the second eq $x_2 = -13/2$. However this makes the third eq. False.

This system is 'inconsistant'. Another way to think about it is that it is <u>overdetermined</u>.

We have a system $A\vec{x} = \vec{b}$ where $\vec{b}$ is not in Col A.

Well, what are we to do? In lieu of finding an exact solution, we may content ourselves with finding the "closest" solution – i.e. the element $\hat{x}$ in Col A ~~for~~ which $A\hat{x}$ is closer to $\vec{b}$ than any other $A\vec{x}$ in Col A.



What do we mean by close? This can be measured is different ways but one of the most common (and intuitive) was is to use least-squares. Let A be an $m \times n$ matrix. Then

$\|\vec{b} - A\vec{x}\|$ is the distance between $A\vec{x}$ and $\vec{b}$ and $\|\vec{b} - A\vec{x}\|^2$ is the square of this distance.

$$\|\vec{b}-A\vec{x}\|^2 = (\vec{b}-A\vec{x}, \vec{b}-A\vec{x}) = (\vec{b}-A\vec{x})\cdot(\vec{b}-A\vec{x})$$
$$= \vec{b}\cdot\vec{b} - 2\vec{b}\cdot(A\vec{x}) + (A\vec{x})\cdot(A\vec{x})$$

If we want to minimize this, we proceed by taking n partial derivatives, $\frac{\partial}{\partial x_i}$, one for each element in $\vec{x}$. Then set these quantities equal to zero.

$$\frac{\partial}{\partial x_i}\left[\vec{b}\cdot\vec{b} - 2\vec{b}\cdot(A\vec{x}) + (A\vec{x})\cdot(A\vec{x})\right] = 0$$

$$0 - 2\vec{b}\cdot(A\vec{e}_i) + \underbrace{(A\vec{e}_i)\cdot(A\vec{x}) + (A\vec{x})\cdot(A\vec{e}_i)}_{\text{Product rule}} = 0$$

because $\frac{\partial}{\partial x_i}\vec{x} = \vec{e}_i$. Since $A\vec{e}_i = \vec{a}_i$ we have

$$-2\vec{b}\cdot\vec{a}_i + 2\vec{a}_i\cdot(A\vec{x}) = 0$$

or

$$\vec{a}_i^T\vec{b} - \vec{a}_i^T A\vec{x} = 0$$

Since this holds for every column $\vec{a}_i$ of A we have

$$A^T\vec{b} - A^TA\vec{x} = 0 \quad \text{or} \quad \boxed{A^TA\hat{x} = A^T\vec{b}}$$

We have switched from $\vec{x}$ to $\hat{x}$ to indicate that this solution is the "best" solution.

These are called the <u>Normal Equations for $\hat{x}$</u>.

<u>Ex.</u> Find the least-squares solution to $A\vec{x}=\vec{b}$ if

$$A=\begin{bmatrix}2&0\\1&1\\1&2\end{bmatrix} \qquad \vec{b}=\begin{bmatrix}7\\-3\\1\end{bmatrix}.$$

$$A^TA=\begin{bmatrix}2&1&1\\0&1&2\end{bmatrix}\begin{bmatrix}2&0\\1&1\\1&2\end{bmatrix}=\begin{bmatrix}6&3\\3&5\end{bmatrix}$$

$$A^T\vec{b}=\begin{bmatrix}2&1&1\\0&1&2\end{bmatrix}\begin{bmatrix}7\\-3\\1\end{bmatrix}=\begin{bmatrix}12\\-1\end{bmatrix}$$

So $$\begin{bmatrix}6&3\\3&5\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=\begin{bmatrix}12\\-1\end{bmatrix} \rightarrow \hat{x}=\begin{bmatrix}3\\-2\end{bmatrix}$$

Note that $A\hat{x}=\begin{bmatrix}6\\1\\-1\end{bmatrix}$ which closer to $\begin{bmatrix}7\\-3\\1\end{bmatrix}$ than any other vector in Col A.

The <u>least squares error</u> is $\|\vec{b}-A\hat{x}\|$.

$$\|\vec{b}-A\hat{x}\| = \left\|\begin{bmatrix}7\\-3\\1\end{bmatrix}-\begin{bmatrix}6\\1\\-1\end{bmatrix}\right\| = \left\|\begin{bmatrix}1\\-4\\2\end{bmatrix}\right\| = \sqrt{1+16+4} = \sqrt{21}$$

When does $A^T A \hat{x} = A^T \vec{b}$ have a unique solution?

If $A^T A$ ($n \times n$ square) has n linearly independent columns then it will be invertible and $\hat{x} = (A^T A)^{-1} A^T \vec{b}$ has a unique solution

So, when does $A^T A$ have n linearly independent columns?

<u>Thm</u> $A^T A$ is invertible iff A has linearly independent columns.

It is entirely possible to find that the least squares solution will have free variables in it – of course this means that $A^T A$ is not invertible and that A does not have n linearly independent columns.